A bosonic RVB description of doped antiferromagnet

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We propose a theory for doped antiferromagnet based on a *bosonic* resonating-valence-bond (RVB) state with incorporating the phase string effect. Both antiferromagnetic (AF) and superconducting phase transitions occur naturally *within* such a bosonic RVB phase. Two distinct metallic regions – underdoping and optimum-doping – are also found to be a logic consequence, whose unique features explain the recent neutron-scattering measurements in cuprates.

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It is well-known that bosonic RVB state [1,2] has a *unrivaled high precision* in describing the $t-J$ model at no-hole case. A mean-field version [3] of such a bosonic spin description also provides a very convenient mathematical framework. Unfortunately, one soon falls into a stalemate once trying to get into metallic phase — always encountering a spiral instability [4,5] at finite doping.

Recently-revealed phase string effect [6] has shed new light on this dilemma. When a doped hole moves on the spin background, the RVB spin pairs are broken up along the way and then re-paired, thanks to the superexchange coupling. However, such a repairing can never be complete for a quantum spin-1/2 media. A phase string is found [6] to be left on the hole-path which is nonrepairable in low energy states. It indicates that a nontrivial Berry's phase will be acquired by a doped hole which slowly completes a closed-loop motion. Obviously, such a topological effect will be lost if the phase string effect is averaged out locally at each step of hopping, which suggests the spiral phase be an artifact of the inappropriate mean-field treatment.

The phase string effect hidden in the bosonic RVB description implies the conventional slave-fermion formalism [5] of the $t-J$ model is not a proper starting-point. A new *exact* reformulation [6] of the model has been obtained after using a canonical transformation to turn the local phase string effect into an explicit nonlocal topological effect. Such a new representation is believed to be more suitable for a mean-field treatment in both 1D and 2D cases [6]. In this paper, we construct a generalized bosonic RVB mean-field theory based on this new formalism. Main results are summarized in the phase diagram shown in Fig. 1, where $\Delta^s \neq 0$ denotes the bosonic RVB phase which practically covers the whole experimentally interested temperature and doping regime. Two real phase transitions occur at low temperature *on* this bosonic RVB background, which are the insulating antiferromagnetic long range order (AFLRO) and superconducting condensation (SC). The former is due to a Bose condensation (BC) of bosonic spinons and the latter is due to a BC of bosonic holons. A striking feature is that the AFLRO cannot exist in the metallic phase but the spinon BC does persist into an underdoped metallic region, leading to a microscopic charge inhomogeneity. All of these, including the normal state, are controlled by the *single* bosonic RVB order parameter Δ^s, indicating the bosonic RVB pairing to be a crucial driving force responsible for a whole spectrum of anomalies in the doped antiferromagnet. Some peculiar predications of the theory will be compared with the experiments in cuprate superconductors.

The $t-J$ model, $H_{t-J} = H_t + H_J$, may be generally expressed as

$$H_t = -t\sum_{\langle ij\rangle} \hat{H}_{ij}\hat{B}_{ji} + H.c., \tag{1}$$

$$H_J = -\frac{J}{2}\sum_{\langle ij\rangle} \hat{\Delta}^s_{ij}\left(\hat{\Delta}^s_{ij}\right)^\dagger. \tag{2}$$

In the Schwinger-bonson, slave-fermion representation [5], one has $\hat{H}_{ij} = f_i^\dagger f_j$, $\hat{B}_{ji} = \sum_\sigma \sigma b^\dagger_{j\sigma} b_{i\sigma}$, and $\hat{\Delta}^s_{ij} = \sum_\sigma b_{i\sigma}b_{j-\sigma}$. Here f_i is a fermionic "holon" operator and $b_{i\sigma}$ is known as the Schwinger-boson operator. The bosonic RVB order parameter first introduced by Arovas and Auerbach [3] is defined as follows

$$\Delta^s = \langle \hat{\Delta}^s_{ij}\rangle. \tag{3}$$

The sign σ appearing in $\hat{B}_{ji}$ is the source of phase string effect mentioned at the beginning. In order to gain a finite hopping integral, i.e., $\langle \hat{B}_{ji}\rangle \neq 0$, at the mean-field level, we see that up and down spins have to contribute differently to avoid cancellation, which always leads to a spiral twist. According to previous discussion [6], however, this mean-field procedure in doped case may be fundamentally flawed as the nontrivial topological effect of phase string is totally lost. To avoid this difficulty, by a canonical transformation [6], one may reformulate the model such that $\hat{B}_{ji} = \sum_\sigma e^{i\sigma A^h_{ji}} \bar{b}^\dagger_{j\sigma}\bar{b}_{i\sigma}$, where the singular sign σ is replaced by a link variable $e^{i\sigma A^h_{ji}}$. Correspondingly, $\hat{\Delta}^s_{ij}$ and $\hat{H}_{ij}$ are redefined by $\hat{\Delta}^s_{ij} = \sum_\sigma e^{-i\sigma A^h_{ij}}\bar{b}_{i\sigma}\bar{b}_{j-\sigma}$ and $\hat{H}_{ij} = e^{iA^f_{ij}} h_i^\dagger h_j$, respectively. Here the nonlocal gauge field A^h_{ij} is defined by a gauge-invariant condition $\sum_C A^h_{ij} = \pi N^h_C$ for an oriented

closed-path C with N_C^h being the total hole number enclosed by C. Apparently A_{ij}^h vanishes at zero-hole limit. And A_{ij}^f satisfies $\sum_C A_{ij}^f = \pi \sum_\sigma \sigma \sum_{l\in C} n_{l\sigma}^b - \Phi_C$ with $n_{l\sigma}^b = \bar{b}_{l\sigma}^\dagger \bar{b}_{l\sigma}$ and Φ_C referring to a uniform flux with a strength of π-per-plaquette enclosed by C. Here new spinon and holon operators, $\bar{b}_{i\sigma}$ and h_i, are both *bosonic* as a peculiar result of the phase string effect.

Now the phase string effect is precisely tracked through the link variables, $e^{i\sigma A_{ij}^h}$ and $e^{iA_{ij}^f}$, in $\hat{B}$, $\hat{\Delta}^s$, and $\hat{H}$. We will still consider the mean-field solution characterized by the RVB order parameter defined in Eq. (3). Similar to the no-hole case [3], the spin part will be diagonalized by a Bogolubov transformation

$$\bar{b}_{i\sigma} = \sum_m \left(u_m \gamma_{m\sigma} - v_m \gamma_{m-\sigma}^\dagger \right) e^{i\sigma\chi_m} \bar{w}_{m\sigma}(i). \qquad (4)$$

Here $\gamma_{m\sigma}$ is an annihilation operator of spinon excitations and the "single-particle" eigenfunction $\bar{w}_{m\sigma}(i)$ is determined by

$$\xi_m \bar{w}_{m\sigma}(i) = -J_s \sum_{j=nn(i)} e^{i\sigma A_{ij}^h} \bar{w}_{m\sigma}(j), \qquad (5)$$

with $J_s = J\Delta^s/2$. We explicitly introduce a phase factor $e^{i\sigma\chi_m}$ in Eq. (4) to show a phase uncertainty in $\bar{w}_{m\sigma}$ which cannot be determined by Eq.(5) as it is a linear equation. It means that the relation between $\bar{b}$ and γ is not unique. Without changing Δ^s, such a "phase" freedom can only be fixed by optimizing the hopping integral $\langle \hat{B}_{ji} \rangle$. Suppose χ_m be a general function of the hole configuration. Then a maximum hopping $\langle \hat{B}_{ji} \rangle$ may be achieved by a simple phase shift $e^{i\sigma\chi_m} \to -sgn(\xi_m) e^{i\sigma\chi_m}$ each time a hole changes a site [7]. The coefficient u_m and v_m in Eq.(4) are given by $(\lambda_m/E_m + 1)^{1/2}/\sqrt{2}$ and $sgn(\xi_m)(\lambda_m/E_m - 1)^{1/2}/\sqrt{2}$, respectively. Here the spinon spectrum is $E_m = \sqrt{\lambda_m^2 - \xi_m^2}$, in which the hopping term only contributes to a shift to the Lagrangian multiplier λ as $\lambda_m = \lambda - J_h/J_s|\xi_m|$. Here the renormalized coupling constant $J_h = \langle \hat{H} \rangle t$ will be always chosen as $J_h = \delta J$ below (δ is the doping concentration). λ is determined by the condition $\sum_i \langle b_{i\sigma}^\dagger b_{i\sigma} \rangle = N(1-\delta)$, or

$$2 - \delta = \frac{1}{N} \sum_m \frac{\lambda_m}{E_m} \coth \frac{\beta E_m}{2} + n_{BC}^b, \qquad (6)$$

where $\beta = 1/k_B T$ and n_{BC}^b represents the number of spinons per site staying at $E_m = 0$ state if a Bose condensation of spinons occurs. In Fig. 1, the region of a nonzero Δ^s is shown which is self-consistently determined after A_{ij}^h in Eq.(5) is approximately replaced by a mean-field $\bar{A}_{ij}^h$ defined by $\sum_C \bar{A}_{ij}^h = \pi \langle N_c^h \rangle$. The effect of fluctuations in A_{ij}^h will be discussed below.

In the bosonic RVB description, Δ^s does not directly correspond to an energy gap, in contrast to the fermionic RVB state [8]. In fact, the spinon spectrum E_m is known [3] to be *gapless* at zero doping and zero temperature which ensures a BC of spinons. In the new formulation, the transverse spin operator can be written as [6]

$$S_i^+ = \bar{b}_{i\uparrow}^\dagger \bar{b}_{i\downarrow} (-1)^i e^{i\Phi_i^h} \qquad (7)$$

in which

$$\Phi_i^h = \sum_{l\neq i} \mathrm{Im}\ \ln\ (z_i - z_l) n_l^h, \qquad (8)$$

describes vortices (with vorticity = 1) centered on holes ($n_l^h = h_i^\dagger h_i$). In the absence of holes, a Bose condensation of spinons will always give rise to $\langle S_i^+ \rangle \propto (-1)^i$, i.e., an AFLRO. But in the presence of mobile holons — in a metallic region — free vortices introduced by Φ_i^h will generally make $\langle S_i^+ \rangle = 0$ even though spinons may be still Bose-condensed, resembling a disordered phase in the Kosterlitz-Thouless transition. Only in an insulating phase where holes are localized, the AFLRO may be still sustained as the vortex effect of Φ_i^h in Eq. (7) can be "screened" through the compensation of a phase with opposite vorticities generated from spinons (After all, the phase string effect is no longer effective if holes are localized).

So the AFLRO should be absent in the metallic phase even though the spinon BC may persist in. One may then wonder what is the nature of such a metallic phase. In the following, we argue that a spinon BC phase in a metallic regime must be generally charge inhomogeneous. Recall that in the BC phase, λ takes a value to make E_m gapless such that $n_{BC}^b \neq 0$ can balance the difference between the left and right sides of Eq.(6). Note that the $E_m = 0$ state corresponds to the maximum of $|\xi_m|$, and thus it is related to those states at the band edge of ξ_m which is generally sensitive to the fluctuation of A_{ij}^h. As A_{ij}^h is basically controlled by the holon density, the fluctuations of the charge will then leads to a "Lifshitz" tail in ξ_m and play an essential role in determining the $E_m = 0$ state, which becomes a macroscopic state after the spinon Bose condensation. Such a state is generally associated with inhomogeneous hole configurations with the condensed spinons forming order in hole-deficient region. Obviously, the detailed nature of the $E_m = 0$ state will be sensitive to many factors, like the dynamics of holons which is beyond the present approximation. We will simply treat the fluctuation part $\delta A_{ij}^h = A_{ij}^h - \bar{A}_{ij}^h$ in terms of a random flux description below. Those quantities like transition temperature T_{BC} will not be our primary concern here. Generally speaking, with the increase of doping, the reduction of the left-hand-side of Eq.(6) will eventually make the BC contribution go away. In Fig.1 the shaded curve sketches such a BC region which basically defines an underdoped metallic phase. (The dotted curve in Fig. 1 marks the insulating AFLRO phase in the dilute hole regime.)

On the other hand, the superconducting order parameter $\hat{\Delta}^{SC}_{ij} = \sum_\sigma \sigma c_{i\sigma} c_{j-\sigma}$ can be expressed [6] in the following form

$$\hat{\Delta}^{SC}_{ij} = \hat{\Delta}^s_{ij} \left(h^\dagger_i e^{\frac{i}{2}[\Phi^s_i - \phi^0_i]} \right) \left(h^\dagger_j e^{\frac{i}{2}[\Phi^s_j - \phi^0_j]} \right) (-1)^i, \quad (9)$$

where

$$\Phi^s_i = \sum_{l \neq i} \text{Im ln } (z_i - z_l) \sum_\alpha \alpha n^b_{l\alpha} \quad (10)$$

describes vortices (anti-vortices) centered on up (down) spinons, and $\phi^0_i \rightarrow \phi^0_i \pm 2\pi$ after i circles once along the loop of a plaquette. In the present bosonic RVB description, spinons are always paired ($\Delta^s \neq 0$). In order to have a superconducting condensation, then, bosonic holons have to undergo a Bose condensation. The vortices described by Φ^s_i are all paired up in the ground state whose effect is minimal there. But at finite temperature, free vortices appear in Φ^s_i as spinons are thermally excited from the paired state. In order to achieve the phase coherence in Eq.(9), the condensed holons have to "screen" those free vortices by forming supercurrents. A phase transition to normal state eventually happens when such "screening" fails which can be estimated as the free spinon number exceeds the holon number. The BC of holons will be interrupted simultaneously. So the transition temperature T_c may be determined by

$$\frac{1}{N} \sum_m \frac{\lambda_m}{E_m} \sum_\sigma \langle \gamma^\dagger_{m\sigma} \gamma_{m\sigma} \rangle \bigg|_{T=T_c} = \kappa\delta, \quad (11)$$

where $\kappa \sim 1$ and the left-hand-side represent the number of excited spinons determined from $\sum_{i\sigma} b^\dagger_{i\sigma} b_{i\sigma}$. T_c calculated based on Eq.(11) is plotted in Fig. 1 as the dashed curve which is obtained under $A^h_{ij} \approx \bar{A}^h_{ij}$ in Eq.(5). This replacement should be considered to be an "optimum" case as the fluctuations of A^h_{ij} generally reduces T_c. We will further discuss the optimum condition later. Finally, the symmetry of the SC order parameter may be determined as

$$\langle \hat{\Delta}^s_{ii+\hat{x}} \rangle / \langle \hat{\Delta}^s_{ii+\hat{y}} \rangle = e^{-i\frac{1}{2}\sum_\Box \Delta\phi^0_{jk}} = -1, \quad (12)$$

where $\sum_\Box$ denotes a summation of $\Delta\phi^0_{jk} \equiv \phi^0_j - \phi^0_k$ over four links of a plaquette and the result indicates a d-wave symmetry for the nearest-neighboring SC pairing.

Therefore, generally there are two temperature scales: T_{BC} and T_c, in a metallic phase. At low doping where $T_{BC} > T_c$, the charge inhomogeneity phase happens below T_{BC} and further below T_c holons are also expected to be condensed into non-uniform regions in favor of the spin correlation energy. On the contrary, once $T_c > T_{BC}$, holons will experience Bose-condensation *first* and be *uniformly* distributed in real space since there is no preformed local spin ordering. Consequently, A^h_{ij} may be replaced by $\bar{A}^h_{ij}$ with a substantial reduction of δA^h_{ij} below T_c. In turn, the spinon spectrum is qualitatively changed which prevents spinons from a Bose condensing into an inhomogeneous phase at low-temperature (see below). T_c shown in Fig. 1 is estimated under such a condition and it optimizes T_c as compared to the case with stronger fluctuations in A^h_{ij}. Beyond $T_c > T_{BC}$, a crossover due to statistics transmutation may quickly set in as holons tend to be *always* Bose-condensed even at high temperature such that spinons have to be turned into fermions, which leads to the breakdown of the bosonic RVB state and is beyond the scope of the present paper.

How can two regions of metallic phase be distinguished by experiment? The underdoped metallic region with a spinon BC must be a charge inhomogeneity phase and also bears some resemblance to "pseudo-gap" phenomenon. For example, both uniform spin susceptibility and transport resistivity will exhibit "pseudo-gap" behavior in this region. But we would like to focus on a more direct experimental signature here. The underdoped phase may be best characterized by a double-peak structure in low-energy region of local dynamic spin susceptibility $\chi''_L(\omega)$ shown in Fig. 2. Here

$$\begin{aligned}\chi''_L(\omega) = \frac{\pi}{4} \sum_{mm'} K_{mm'} \, [1/2(1 + n(E_m) + n(E'_m)) \\ \cdot(u^2_m v^2_{m'} + v^2_m u^2_{m'})\delta(|\omega| - E_m - E_{m'}) + (n(E_m) \\ -n(E_{m'}))(u^2_m u^2_{m'} + v^2_m v^2_{m'})\delta(\omega + E_m - E_{m'})] \, , \quad (13)\end{aligned}$$

where $\omega > 0$ with $K_{mm'} \equiv \sum_{i\sigma} |w_{m\sigma}(i)|^2 |w_{m'\sigma}(i)|^2$ and $n(E_m)$ as the Bose function. The lowest peak in Fig. 2 originates from excitations from the condensed spinons which can be explicitly sorted out from Eq.(13) as

$$\chi''_c(\omega) = \left(\frac{\pi}{4} n^b_{BC} \right) \sum_m K_{0m} \frac{\lambda_m}{E_m} \delta(\omega - E_m), \quad (14)$$

where $m = 0$ refers to the BC state. This peak disappears above T_{BC}, while the second peak is contributed by usual spinon pairs excited from the vacuum. Here δA^h_{ij} is treated as a random flux, as noted before, with a strength of the flux per plaquette $\delta\phi = 0.3\pi\delta$ at $\delta = 1/7 \approx 0.143$. Corresponding T_{BC} is found to be $\sim 0.21J$. In contrast, if the holon BC happens first such that $A^h_{ij} \approx \bar{A}^h_{ij}$, then the spinon BC is found absent below T_c and only a single peak is left as shown in the insert of Fig. 2. Note that the sharpness of the peak is due to the Landau-level effect caused by $\bar{A}^h_{ij}$ in E_m (for simplicity we choose $\delta\phi = 0$ here, i.e., δA^h_{ij} is totally neglected below T_c). Other choices of parameters all yield similar two types of structure depending only on whether there is a spinon BC or not.

Neutron-scattering measurement has indeed revealed a double-peak structure in $YBa_2Cu_3O_{6.5}$ compound recently [9], where the lower peak is located near $30meV$ and the second one is, around $60meV$, about twice bigger in energy as predicted by the theory (Fig. 2). Thus, this

underdoped material can be understood in the present theory as in the spinon BC phase. On the other hand, a "resonance-like" sharp peak at $41meV$ has been well-known for $YBa_2Cu_3O_7$ below T_c [10], which is consistent with the case shown in the insert of Fig. 2 if $J \sim 100meV$. Namely, it corresponds to the uniform phase without the spinon BC, defined as an optimum metallic region in the theory with an optimized T_c. A single peak located at $\mathbf{Q}_0 = (\pi, \pi)$ is also identified in the momentum space at the "resonance" energy in both the experiment and theory, suggesting an AF nature of spin fluctuations. But an incommensurate momentum structure is generally present at energy near the first peak shown in Fig. 2 in the spinon BC phase with charge inhomogeneity, which is sensitive to the nature of the BC state. Finally, it is noted that in the bosonic RVB description, the double-layer coupling should not qualitatively change the above energy structure in the odd symmetry channel.

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[1] S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).

[2] Y.-C. Chen and K. Xiu, Phys. Lett. B**181**, 373 (1993); Y. -C. Chen, Mod. Phys. Lett. B**8**, 1253 (1994).

[3] D.P. Arovas and A. Auerbach, Phys. Rev. B**38**, 316 (1988).

[4] B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **62**, 1564 (1989); **61**, 467 (1988).

[5] C. Jayaprakash *et al.*, Phys. Rev. B **40**, 2610 (1989); D. Yoshioka, J. Phys. Soc. Jpn., **58**, 1516 (1989); C. L. Kane *et al.*, Phys. Rev. B**41**, 2653 (1990); Z. Y. Weng, Phys. Rev. Lett. **66**, 2156 (1991).

[6] D. N. Sheng, Y. C. Chen, and Z. Y. Weng, Phys. Rev. Lett. **77**, 5102 (1996); Z. Y. Weng, D. N. Sheng, Y. C. Chen, and C. S. Ting, Phys. Rev. B**55**, 3894 (1997).

[7] Z. Y. Weng, D. N. Sheng, and C. S. Ting, unpublished.

[8] P. W. Anderson, Science **235**, 1196 (1987); G. Baskaran *et al.*, Solid State Comm. **63**, 973 (1987).

[9] P. Bourges, *et al.*, preprint, cond-mat/9704073.

[10] H. F. Fong, *et al.*, Phys. Rev. Lett. **75**, 316 (1995); M. A. Mook, et al., Phys. Rev. Lett. **70**, 3490 (1990)

Fig. 1 The phase diagram of doped-antiferromagnet based the bosonic RVB description. The dotted and shaded curves sketch an insulating AFLRO phase and an inhomogeneous metallic region, respectively, described by a spinon Bose condensation (BC). SC indicates the superconducting condensation region determined under an optimal condition (see the text). The temperature T is in units of J.

Fig. 2 Local dynamic spin susceptibility $\chi''_L(\omega)$ vs. ω (in units of J) at $\delta = 0.143$. Solid curve: $T = 0$; ($\diamond$): $T = 0.1$; ($\times$): $T = 0.2$; ($*$): $T = 0.3$. Here $T_{BC} = 0.21$ with $\delta\phi = 0.3\bar{\phi}$. The insert: $\chi''_L(\omega)$ vs. ω under the optimal condition: $\delta\phi = 0$ at $T = 0$.

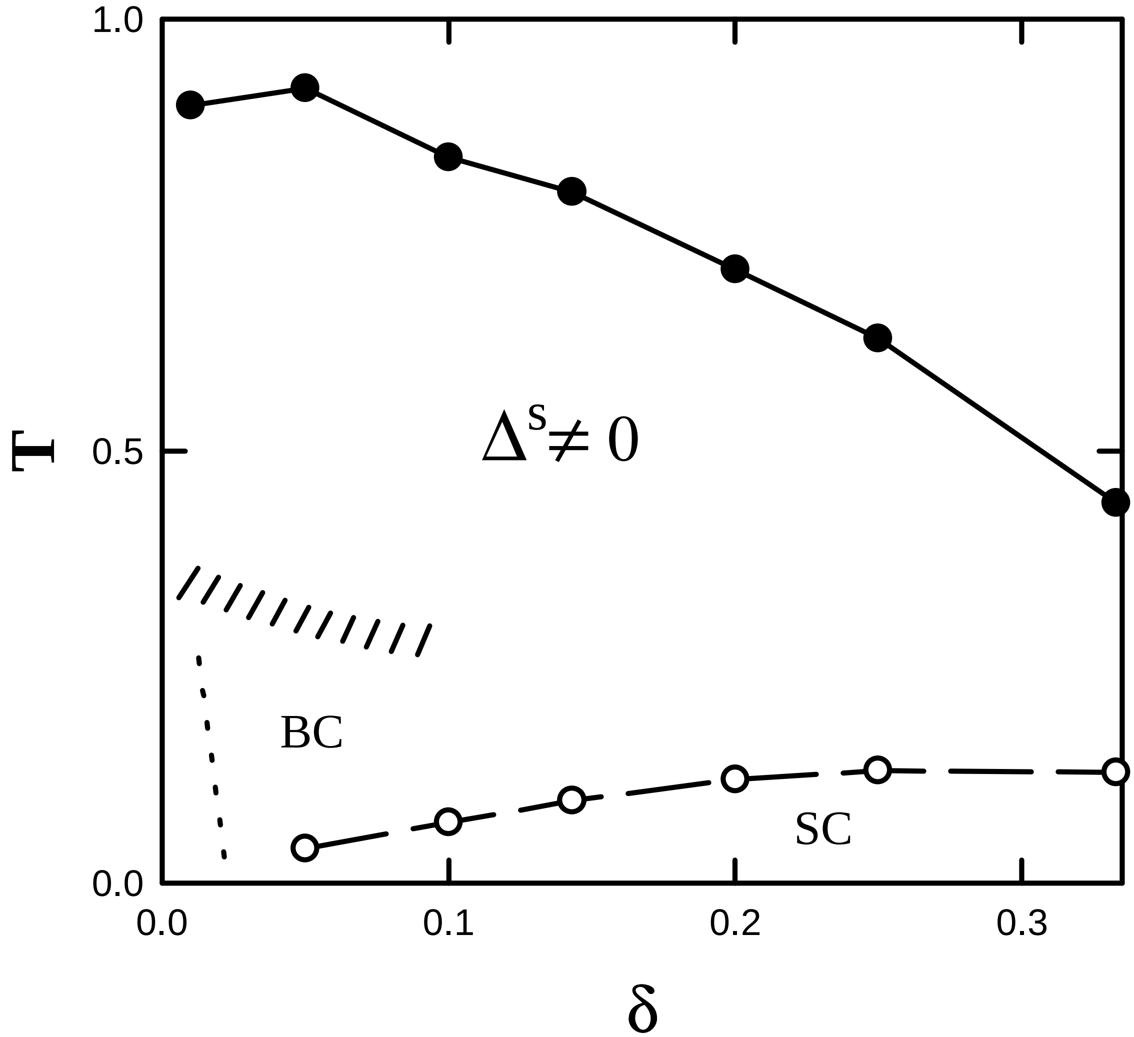
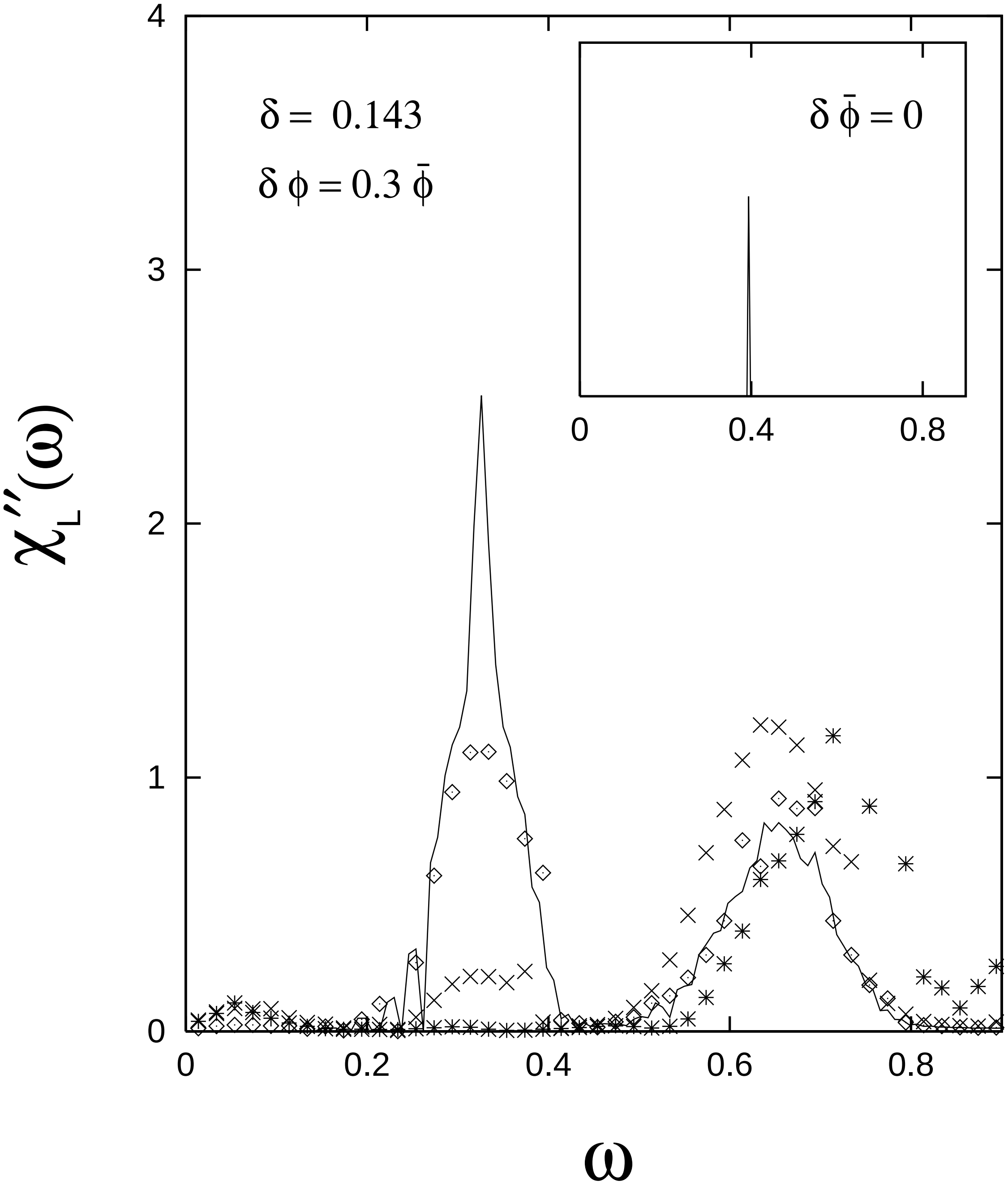


Fig. 1



$\delta = 0.143$
$\delta\phi = 0.3\,\bar{\phi}$
$\delta\bar{\phi} = 0$
$\chi_L''(\omega)$
ω
0
1
2
3
4
0
0.2
0.4
0.6
0.8
0
0.4
0.8

Fig. 2